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SOFTWARE FOR THE IMPEDANCE ANALYSIS OF CERAMIC DIELECTRICS

T.A. Wheat, A. Ahmad and J.D. Canaday
Mineral Processing Laboratory

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SOFTWARE FOR THE IMPEDANCE ANALYSIS OF CERAMIC DIELECTRICS

by

T.A. Wheat*, A. Ahmad** and J.D. Canaday**

ABSTRACT

The present authors have previously described a computer-controlled system for the electrical characterization of ceramic dielectrics based on a low-cost controller and software driving a Hewlett-Packard HP4192A spectral impedance analyser.

The present report describes additional routines which enable the operator to view the data graphically, to select appropriate portions of the data and to obtain a least-squares regression fit of a series of near semi-circles through those selected portions. The program reports the relative error of the best fit circle through the data, the maximum value of Y, the two values of X when the fitted arc is extrapolated to Y=0 and the so-called 'depressed angle' formed between the X-axis and the circle radius drawn between the circle centre and the point {0,0}.

The operator can elect to erase the fitted data at any time and try other segments of the data range to obtain a minimum relative error. The original data and the fitted data may be stored on disc separately for later use in commercial graphics programs producing camera-ready figures.

Keywords: Software, Impedance analysis, Ceramic Dielectrics, Electrical characterization.

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* Head and ** Research Scientist, Ceramics Section, Mineral Processing Laboratory, Mineral Sciences Laboratories, CANMET, Energy, Mines and Resources Ottawa, Canada.

DÉVELOPPEMENT D'UN LOGICIEL POUR L'ANALYSE DE L'IMPÉDANCE DES MATÉRIAUX CÉRAMIQUES DIÉLECTRIQUES

par

T.A. Wheat*, A. Ahmad** et J.D. Canaday**

RÉSUMÉ

Les auteurs de ce rapport ont déjà donné une description d'un système assisté par ordinateur utilisé pour la caractérisation électrique des matériaux céramiques diélectriques. Le système était doté d'un analyseur de spectre Hewlett-Packard HP4192A pour l'analyse de l'impédance, commandé par une unité de contrôle et un logiciel peu coûteux.

Le présent rapport comprend une description des programmes supplémentaires qui permettent à l'opérateur de représenter les données sous forme de graphique, de choisir les portions de données appropriées et d'obtenir le calage par moindres carrés de la régression d'une série de quasi semi-cercles au moyen des données sélectionnées. Le programme signale l'erreur relative du cercle dont l'ajustage est le plus juste, au moyen des données, la valeur maximale de Y, les deux valeurs de X quand l'arc ajusté est extrapolé à Y=0 et que le soit-disant "angle de dépression" se soit formé entre l'axe X et le rayon du cercle tiré à partir du centre du cercle et du point {0,0}.

L'opérateur peut choisir d'effacer les données ajustées en tout temps et essayer d'autres tranches de données en vue d'obtenir un taux d'erreur relatif minimal. Les données initiales et les données ajustées peuvent être enregistrées séparément sur un disque pour utilisation future dans des programmes graphiques commerciaux qui produisent des figures prêtes à photographier.

Mots-clé : Logiciel, analyse de l'impédance, matériaux céramiques diélectriques, caractérisation électrique.

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* Chef et ** Chercheur scientifique, Section de la céramique, Laboratoire de traitement des minéraux, Laboratoires des sciences minérales, CANMET, Énergie, Mines et Ressources, Ottawa, Canada.

INTRODUCTION

For many years, the Ceramics Section has been involved in all aspects of the development of a wide range of electrical ceramics ranging from a variety of non-conducting polycrystalline piezoelectrics to a number of highly conducting solid electrolytes. In all cases, the work has centred on the iterative process of synthesizing the materials and determining the properties of the finished product. As the electrical characterization yields much useful information concerning the quality of the product and the direct effect of various processes on the behaviour of the material, it is an essential tool in the development of dielectric materials.

The analysis of the electrical properties of ceramic materials and the determination of the contributions from the grain and grain-boundary regions of the ceramic as well as the surface electrodes commonly depends on modelling the electrical response of the sample over a range of frequencies to that of resistor-capacitor networks in various configurations. Similar modelling is also used to analyse electrode-ceramic behaviour in systems such as sensors, batteries, fuel cells, transducers, etc. In practice, the behaviour of a material is most conveniently determined using an impedance spectral analyser such as a Solartron 1172 or a Hewlett-Packard HP-4192A as part of a computer-controlled system that allows the real and imaginary impedance to be measured over a range of frequencies {typically 100 Hz to 1 MHz} at a given temperature in the range from -180C to 800C. In this way, the data can be acquired and manipulated automatically.

The authors have previously reported on the implementation of such a system based on an Apple IIe controller driving a HP-4192A Impedance Analyser and gave examples of the characterization of piezoelectric ceramics driven through resonance so that the sample capacitance, coupling factor, loss and dissipation could be determined {1}. The system has also been used to characterize a number of solid electrolytes either as simple discs held between blocking electrodes or as the membrane of hydrogen-air fuel cell employing non-blocking electrodes.

The dispersion and absorption that occurs in dielectric materials under an alternating field has continued to be studied extensively since the classical treatment of polar liquids by Debye in 1929 who showed that the electrical behaviour can be modelled entirely by RC networks resulting in the locus of the complex dielectric constant forming a perfect semi-circle in the complex plane {4}, Fig. 1{a}. Later, Cole and Cole were to show that many real materials deviated from this ideal Debye behaviour such that the resistive component of Fig. 1{a} is replaced by a complex impedance Z {Fig. 1{b}:

$$Z = \tau_0(i\omega\tau_0)^{-\alpha}/(\varepsilon_0 - \varepsilon_\infty)$$

so that the locus of the complex dielectric constant now forms an arc in the complex plane, i.e., the original semi-circle is depressed {5}. They noted that although the reactive component of the impedance is frequency dependent, the phase angle is frequency independent and is equal to alpha x pi/2 which is also the magnitude of the angle between the epsilon' axis and the circle radius between $\text{epsilon}_{\text{infinity}}$ and the circle centre, Fig. 1{b}.

More recently, Bauerle appears to be the first to apply this technique in his study of solid electrolytes {6} noting that the use of a very small ac current through the material and measurement of the impedance {or admittance} with frequency will not only avoid irreversible electrode changes and heating effects but will allow resolution of the various polarization effects occurring in the both the sample and at the sample-electrode interface. In his study of the behaviour of yttria-stabilized zirconia solid electrolytes between blocking Pt electrodes in the temperature range 400-800°C, he was able to isolate the components of the various polarizations that occurred illustrating the power of the technique.

Since the mid 1970's, the technique has become more widely used, particularly in the analysis and characterization of a wide range of solid electrolytes and it has become increasingly apparent that the resolution of distinct semi-circles that characterized the earlier work was more the exception than the rule. Schouler was among the first to show the progressive merging of semi-circles which is observed in doped thoria - with a reduction in dopant levels, the semi-circles merge so that at low levels it is impossible to visually distinguish the component semi-circles {7}.

Recently, Kleitz and Kennedy have proposed an iterative procedure by which the components of merged semi-circles may be resolved {8}. Essentially, they propose:

{i} using that part of the data set which has minimum overlap {e.g., using the low frequency data only} and calculating the full semi-circle from that limited data;

{ii} determining the difference between the calculated and real data over the full frequency range;

{iii} calculating a second semi-circle using now the high-frequency data set only that remains from step {ii};

{iv} finally the two approximated semi-circles are summed and the average difference between the real and calculated data is determined. The process is iterated to minimize the deviation between the calculated and real data.

However, the authors admit their procedure does require the investigator to make several subjective decisions at various points in the process.

The present authors have used a similar principle - that of using the region of the data with the minimum overlap. However, unlike the iterative averaging use by Kleitz and Kennedy, they have applied a least squares regression analysis to give directly the component semi-circle {or arc in the case of depressed figures} that best fits the data. By presenting a graphical display of the original data and the fitted semi-circle{s} together with the relative error of the regression for each semi-circle, their intercepts of the X axis {real component} at Y=0, the frequency for the maximum value of Y {imaginary component} and the depressed angle, it is possible to rapidly resolve the components of partially overlapping data.

The software allows the raw and fitted data to be stored on disc for later use in commercial graphics programs. The graphics screen may be dumped directly at any time and a printout can be obtained of the semi-circle data following solution of the regression analysis. Although the method is not absolute it does give satisfactory information rapidly and requires minimal judgement on the part of the operator.

The program listed in Appendix A is a stand alone routine to fit a circle through graphically displayed initial data by regression analysis and to report the significant statistics of the fit such as Ymax, the two values of X at Y=0, etc. and to store the fitted data on disc for latter use. The variables used in the routine are identified in Apprendix B. The essence of the routine lies in lines 15000 to 16080 which form the subroutine added to the original program reported elsewhere {1} and not repeated here.

The geometry used to develop the equation for a least-squares regression is given in Fig. 2 and is described below. The principal parameters required of any fitted data are shown in Fig. 3 and the overall flow sheet of the software for the complete program, i.e., the original material reported in {1} together with the circle regression subroutine reported here, is given in Fig. 4.

Figure 5 shows the raw impedance data of an RC network together with the fitted arc as obtained from a graphics dump built into the present subroutine. Figure 6 shows the same data with the fitted curve derived from different segments of the original data set. By saving the fitted data as a separate file in such a manner that it is compatible with existing commercial graphics software , it is possible to create camera-ready material as shown in Fig. 7.

A LEAST SQUARES REGRESSION FIT OF DATA TO A CIRCLE

From Fig. 2, the following equations can be derived:

$$X' = (X_n + X_1)/2$$

$$Y' = (Y_n + Y_1)/2$$

$$M_1 = (Y_n - Y_1)/(X_n - X_1) = -1/M_2$$

It can be seen that in triangle ABD:

Line AB $\quad M_2(X - X') = (Y - Y') \qquad (1)$

Triangle ABD : $\quad Rho^2 = (X - X')^2 + (Y - Y')^2 \qquad (2)$

Subs (1) in (2) $\quad Rho^2 = (X - X')^2 + M_2^2(X - X')^2 \qquad (3)$

From (3) $\quad (X - X') = Rho/SQR(1 + M_2^2) \qquad (4)$

Subs (4) in (1) $\quad (Y - Y') = M_2.Rho/SQR(1 + M_2^2) \qquad (5)$

Similarly, in triangle ACE:

$$R^2 = (X_n - X)^2 + (Y_n - Y)^2 \qquad (6)$$

Subs (4) & (5) in (6)

$$= \left(X_n - X' - \frac{Rho}{SQR(1 + M_2^2)}\right)^2 + \left(Y_n - Y' - \frac{M_2.Rho}{SQR(1 + M_2^2)}\right)^2 \qquad (7)$$

The square of the difference between circle centre to actual datum (d_i) and fitted circle radius r is $(d_i^2 - r^2)^2$

$$= \{[(X_i - X') - Rho/Z]^2 + [(Y_i - Y') - M_2.Rho/Z]^2 - [(X_n - X') - Rho/Z]^2 - [(Y_n - Y') - M_2.Rho/Z]^2\}^2 \quad (8)$$

(where $Z = SQR[1 + M_2^2]$)

The sum of these differences between i=1 to n is $Q = \sum_{i=1}^{n}(d_i^2 - r^2)^2$

Rearrange (8) gives:

$$Q = \sum_{i=1}^{n}\{[(X_i - X') - Rho/Z]^2 - [(X_n - X') - Rho/Z]^2 + [(Y_i - Y') - M_2.Rho/Z]^2 - [(Y_n - Y') - M_2.Rho/Z]^2\}^2 \quad (9)$$

Rearrange (9) gives:

$$Q = \sum_{i=1}^{n}\{(X_i - X_n)(X_i - 2X' + X_N - 2.Rho/Z) + (Y_i - Y_n)(Y_i - 2Y' + Y_n - 2M_2.Rho/Z)\}^2 \quad \ldots (10)$$

Best fit occurs when Q is a minimum, i.e., when the differential d(Q)/d(Rho)=0

$$dQ/d(Rho) = 0 = \sum_{i=1}^{n}2[-2(X_i - X_n)/Z + -2M_2(Y_i - Y_n)/Z] \times [(X_i - X_n)(X_i - 2X' + X_n - 2Rho/Z) + (Y_i - Y_n)(Y_i - 2Y' + Y_n - 2M_2Rho/Z)] \quad (11)$$

Simplified, (11) becomes:

$$0 = \sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]\,[(X_i - X_n)(X_i - 2X' + X_n - 2Rho/Z) + (Y_i - Y_n)(Y_i - 2Y' + Y_n - 2Rho/Z)] \quad (12)$$

Rearrange (12):

$$0 = \sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]\,[(X_i - X_n)(X_i - X') + (Y_i - Y_n)(Y_i - Y')] + \sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]^2\,(-2Rho/Z)] \quad (13)$$

Rearrange (13):

$$2Rho/Z = \frac{\sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]\,[(X_i - X_n)(X_i - X') + (Y_i - Y_n)(Y_i - Y')]}{\sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]^2}$$

$$Rho = \frac{Z\sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]\,[(X_i - X_n)(X_i - X') + (Y_i - Y_n)(Y_i - Y')]}{2\sum_{i=1}^{n}[(X_i - X_n) + M_2(Y_i - Y_n)]^2} \quad \ldots (14)$$

The general equation for any circle is:

$$X^2 + Y^2 = R^2$$

Hence, equation of best fit circle through real (x_i, y_i) data pairs from i=1 to n is given by:

$$\begin{matrix} X^2 & + & Y^2 & = & R^2 \\ (X - X' - Rho/Z)^2 & + & (Y - Y' - M_2Rho/Z)^2 & = & (X_n - X' - Rho/Z)^2 + (Y_n - Y' - M_2Rho/Z)^2 \end{matrix}$$

i.e., for a given value of Y:

$$X = \pm SQR[(X_n - X' - Rho/Z)^2 + (Y_n - Y' - M_2Rho/Z)^2 - (Y - Y' - M_2Rho/Z)^2] + X' (Rho/Z)$$

i.e., $X = T2 \pm T1$ where

$$T1 = SQR[(X_n - X' - Rho/Z)^2 + (Y_n - Y' - M_2Rho/Z)^2 - (Y - Y' - M_2Rho/Z)^2]$$

$$T2 = X' (Rho/Z)$$

The circle radius is given by:

$$Radius = (X_n - X' - Rho/Z)^2 + (Y_n - Y' - M_2Rho/Z)^2$$

and the relative error {E} of the fitted data is given by:

$$E = SQR \{Q\}/nRadius.$$

REFERENCES

1. T.A. Wheat and A. Ahmad "Software for the Electrical Characterization of Ceramics USing an Apple Controller and a Hewlett-Packard 4192A Impedance Analyser", MSL 86-1{IR}

2. A. Ahmad, J.D. Canaday, T.A. Wheat and A.K. Kuriakose, "A Computer Controlled Data Acquisition System for Electrical/Electrochemical Characterization of Ceramics Materials", Jour. Can. Ceram. Soc. 53 8-14 {1984}.

3. J.D. Canaday, T.A. Wheat, A.K. Kuriakose and A. Ahmad, "A Micro-computer System for Fuel Cell Experiments", Jour. Electrochem. Soc. Ext Abs. #376 85-1 538-539 {1985}.

4. P. Debye, "Polar Molecules", pub Chemical Catalogue Co., NY, 1929.

5. K.S. Cole and R.H. Cole "Dispersion and Absorption in Dielectrics I. Alternating Current Characteristics", Jour. Chem. Phys., 9 #4 341-351 {1941}.

6. J.E. Bauerle, "Study of Solid Electrolyte Polarization by a Complex Admittance Method", Jour. Phys. Chem. Solids, 30 2657-2670 {1969}.

7. E. Schouler, A. Hammou and M. Kleitz, "Complex Impedance of Electrochemical Cells Based on Yttria-dopped Thoria", Mat. Res. Bull. 11 1137-1142 {1976}.

8. M. Kleitz and J.H. Kennedy, "Resolution of Multi-component Impedance Diagrams", Proc. Solid Electrolytes 1979 Conf. 185-188 {1979}.

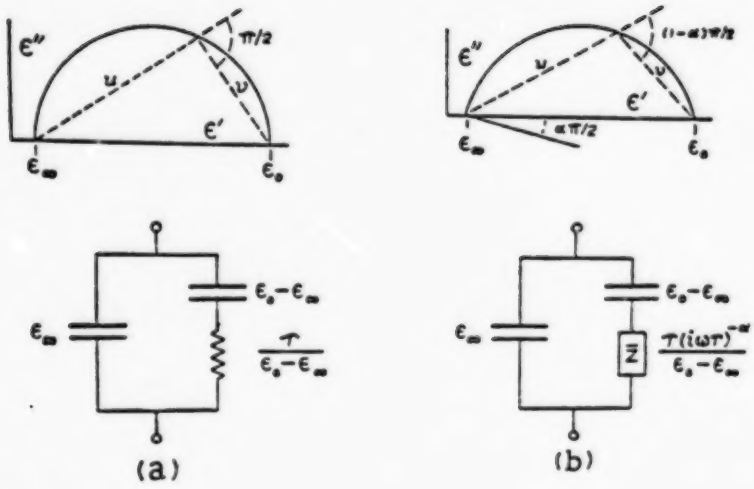


Fig. 1 - Theoretical complex plane loci of the complex dielectric constant of a material together with the equivalent circuits:
{a} Debye theory {full semi-circle}
{b} Experimental evidence {depressed semi-circle}
{After ref 5}.

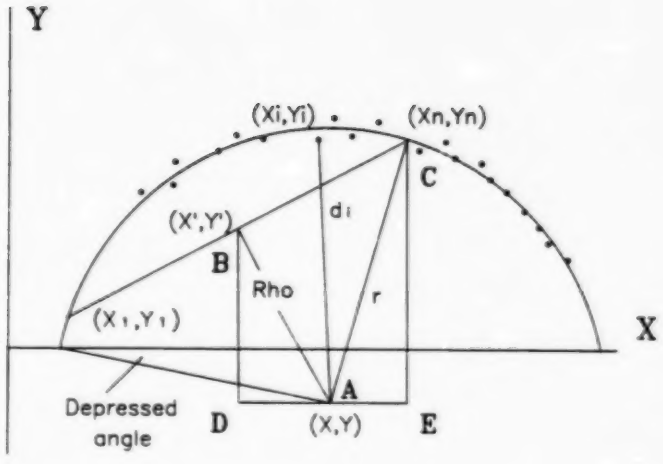


Fig. 2 - Geometry used to develop regression equation to fit an arc through a series of {X,Y} datum points.

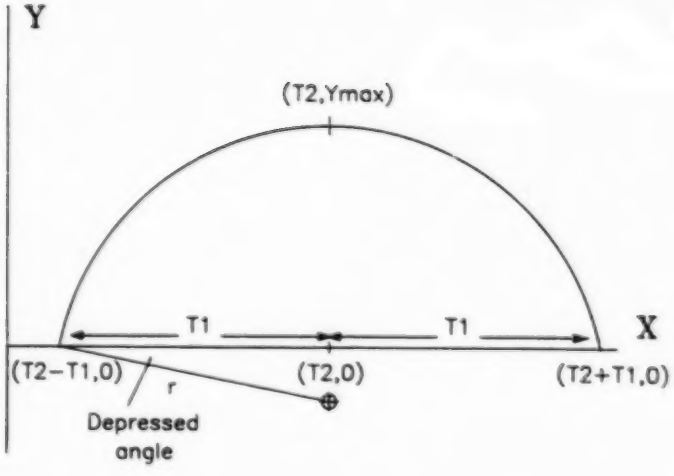


Fig. 3 - Principal parameters required of fitted arc - depressed angle and four {X,Y} co-ordinates

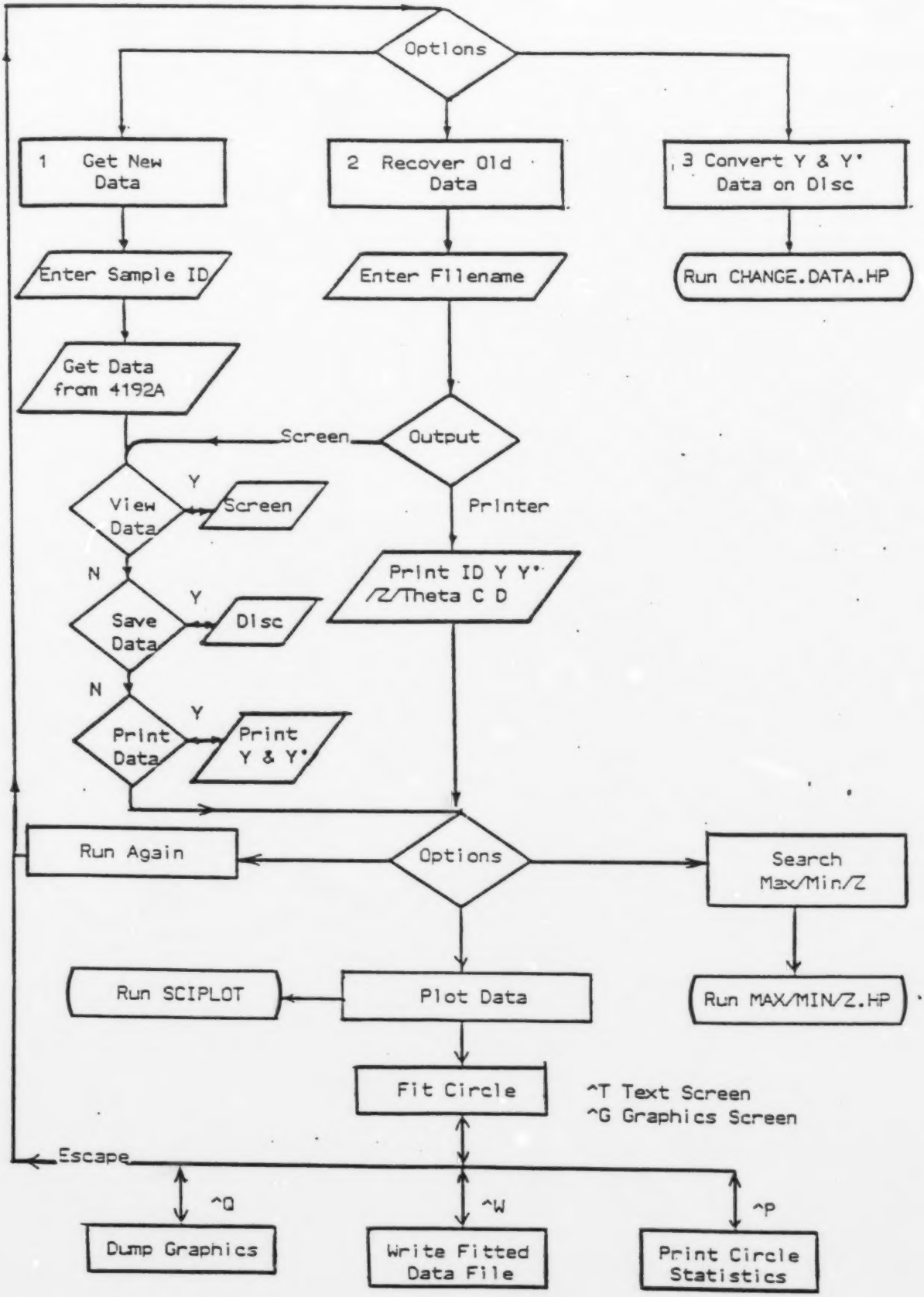
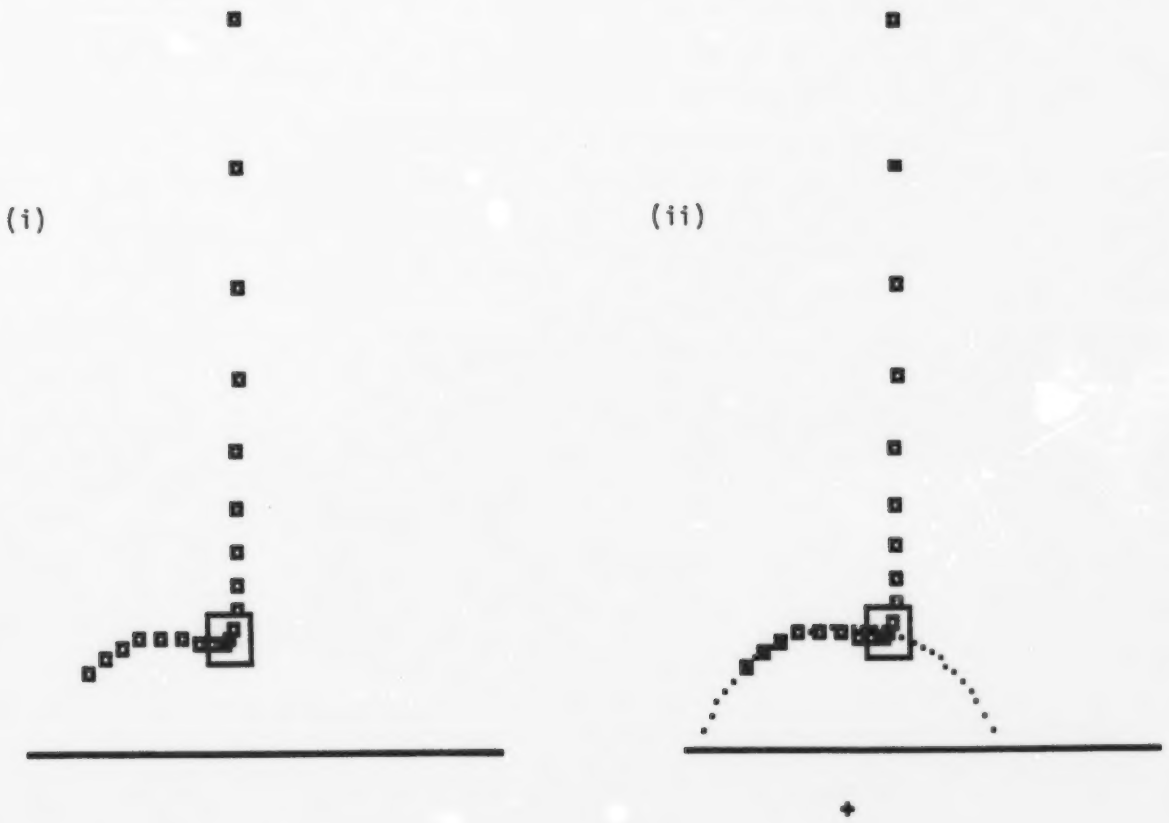


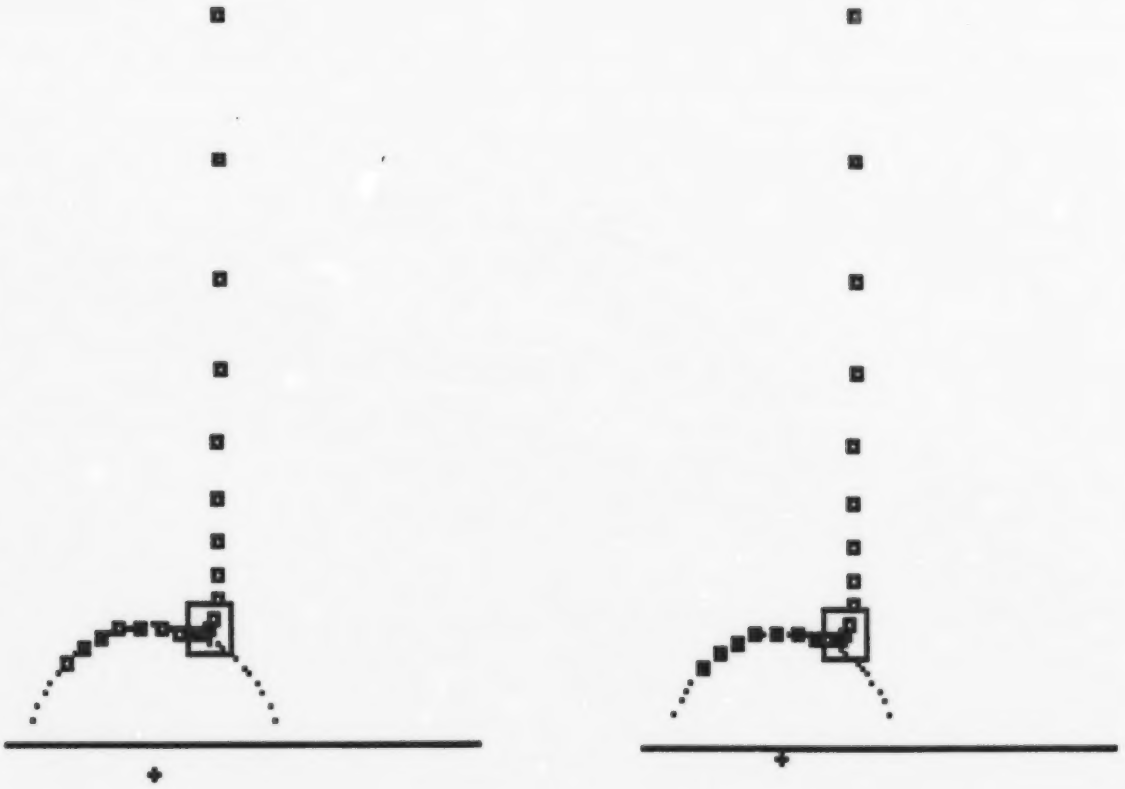
Fig. 4 - Flow sheet for overall program.



File: BOX/1-10KHZ has 22 data points
Used data between points 12 and 22

BULK RES	=	57.0188856
Rb + Rg	=	1622.63031
Radius	=	825.289758
Rel error	=	5.8 %
1/(Rb + Rg)	=	6.16283322E-04
1/Bulk	=	.0175380488
MAX IMAGINARY Z	=	563.911877
FREQ. AT MAX Z	=	35.8970655 KHz
DEPRESSED ANGLE	=	18.4641025 DEG

Fig. 5 - Original data dumped from graphics screen (i) with the first attempt to fit a semi-circle shown in (ii) using data points 12 to 22. An oversized square indicates the mid point of the original array.



File: BOX/1-10KHZ has 22 data points
Used data between points 14 and 22

BULK RES	=	107.258615
Rb + Rg	=	1417.81195
Radius	=	665.958724
Rel error	=	2.4 %
1/(Rb + Rg)	=	7.05312152E-04
1/Bulk	=	9.3232604E-03
MAX IMAGINARY Z	=	547.158436
FREQ. AT MAX Z	=	43.5337311 KHz
DEPRESSED ANGLE	=	10.2759881 DEG

File: BOX/1-10KHZ has 22 data points
Used data between points 16 and 22

BULK RES	=	146.746711
Rb + Rg	=	1312.39737
Radius	=	584.096138
Rel error	=	.5 %
1/(Rb + Rg)	=	7.61964341E-04
1/Bulk	=	6.8144628E-03
MAX IMAGINARY Z	=	545.587285
FREQ. AT MAX Z	=	46.96304 KHz
DEPRESSED ANGLE	=	3.78019341 DEG

Fig. 6 - As for Fig. 5 using progressively higher frequency data and hence less overlap with the low frequency data showing the progressive reduction in the depressed angle and the improvement in the relative error of the fit.

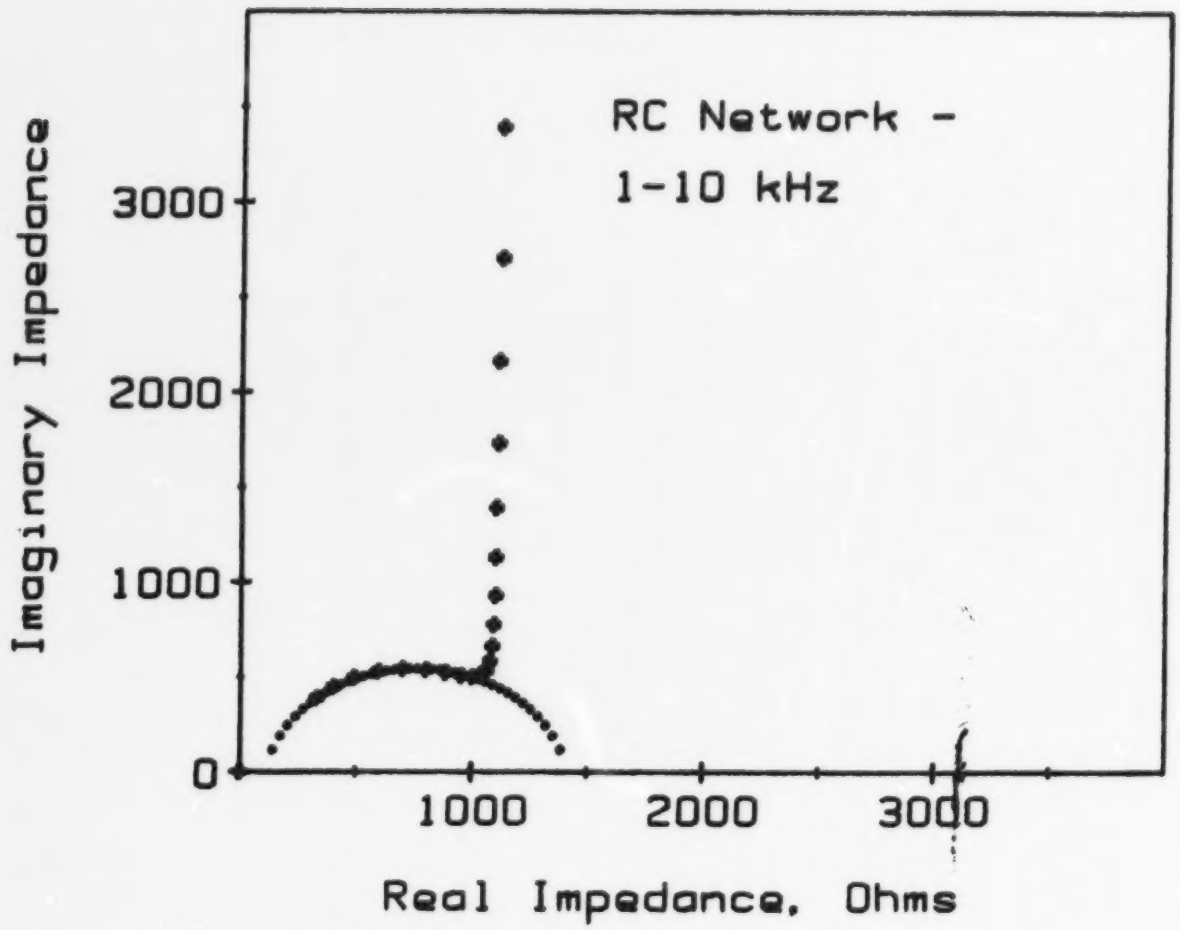


Fig. 7 - Example of final camera-ready figure of original and fitted data obtained using commercial software and a flat-bed plotter.

Appendix A

Software Listing of Subroutine to Generate

Least-squares Regression Analyses of Cole-Cole Plots

Note: The subroutine per se is given betweeen lines 15000 and 16080 - material incorporated prior to 15000 results in a stand-alone program that can recall data from disc, present it graphically and generate a least squares fit through selected points.

```
0  REM  - FILE - CIRCLE LEAST SQUARES 050588
1  REM  +-----------------------------------------------------+
2  REM  |                                                     |
3  REM  |    ROUTINE TO SCALE & PLOT ANY DATA ON THE GRAPHICS |
4  REM  |    SCREEN & TO FIT A CIRCLE THROUGH A SELECTED PART |
5  REM  |    OF THE ORIGINAL PLOT.                           |
6  REM  |                                                     |
7  REM  |    The fitted data can be plotted and erased at will|
8  REM  |   and gives a listing (on screen or printer) of the |
9  REM  |   relative error of the least squares fit, the value|
10  REM |   of Ymax (top of circle), the value of X at Ymax,  |
11  REM |   the values of X for circle when Y=0 and the angle |
12  REM |   between the Xaxis and the circle radius to Y=0 -  |
13  REM |   the depressed angle.                              |
14  REM |                                                     |
15  REM |    When the question "OK (Y/N)" is posed the user   |
16  REM |   can select from the following commands:           |
17  REM |   CTRL-G    switch to graphics screen               |
18  REM |   CTRL-P    direct numerical data to printer        |
19  REM |   CTRL-Q    dump graphics screen on printer         |
20  REM |   CTRL-T    switch to text screen                   |
21  REM |   CTRL-W    write fitted circle (X,Y) data to disc  |
22  REM |               using the original filename with the  |
23  REM |               extension xxx.FIT/n, where n is 1,2,  |
24  REM |               3, etc incremented each time fitted   |
25  REM |               data is saved for the original file   |
26  REM |   ESC       return & input new data to process      |
27  REM |                                                     |
28  REM |   To assist in selecting the points on the screen - |
29  REM |   which can be crowded - an enlarged square is used |
30  REM |   for the middle datum (or one after) point         |
31  REM |                                                     |
32  REM |                      May 1988                       |
33  REM |                                                     |
34  REM +-----------------------------------------------------+
35 :
36  CLEAR
40 :
43  HIMEM: 38399: LOMEM: 26369:D$ =  CHR$ (4): PRINT D$;"PR#0"
44  POKE 232,00: POKE 233,03: IF  PEEK (776) = 35 AND  PEEK (787) = 38 THEN  GOTO 48

46  PRINT D$;"BLOADSHAPES"
47  PRINT D$;"BLOADGRAFPAK.QUICK"
48  DIM D(200),A$(15),X(42),Y(42)
1000 :
1010  REM +-----------------------------------------------+
1020  REM |                                               |
1030  REM |  READ Filename.DATA/.ID Files get data to plot |
1040  REM |                                               |
1050  REM +-----------------------------------------------+
1060 :
1070  HOME : VTAB 10: PRINT "PUT DATA DISK IN DRIVE 2 ... AND HIT ANY KEY ": GET A$
1080  HOME : VTAB 10: PRINT "ENTER FILE NAME": VTAB 12: HTAB 5: INPUT "... .DATA/.ID
      NOT NEEDED ";FI$
1090  PRINT D$;"OPEN";FI$".DATA,D2"
1100  PRINT D$;"READ";FI$;".DATA"
1110  INPUT D(0):D(0) = D(0) - 2: REM  GET # DATA PTS IN FILE AND DISCARD LAST SET
```

```
1120  FOR X = 1 TO D(0)
1130  INPUT D(X)
1140  NEXT X
1150  PRINT D$;"CLOSE";FI$;".DATA"
1160  PRINT D$;"OPEN";FI$;".ID"
1170  PRINT D$;"READ";FI$;".ID"
1180  FOR X = 1 TO 11: REM INFO IN LINES 210-260
1190  INPUT A$(X)
1200  NEXT X
1205 LF =  VAL (A$(9)):MM =  VAL (A$(11))
1210  PRINT D$;"CLOSE";FI$;".ID"
15000 :
15010  REM  +-----------------------------------------------------------------+
15015  REM  |                                                                 |
15020  REM  |  LEAST SQUARES REGRESSSION FIT OF CIRCLE THROUGH SELECTED POINTS |
15025  REM  |                                                                 |
15030  REM  +-----------------------------------------------------------------+
15070 :
15080 X3 = D(1): FOR I = 1 TO D(0) STEP 2
15090  IF  SGN (D(I)) =  - 1 THEN D(I) =  ABS (D(I))
15100  IF D(I) > X3 THEN X3 = D(I): REM   FIND X MAX
15110  NEXT
15120 Y3 = D(2): FOR I = 2 TO D(0) STEP 2
15130  IF  SGN (D(I)) =  - 1 THEN D(I) =  ABS (D(I))
15140  IF D(I) > Y3 THEN Y3 = D(I): REM FIND Y MAX
15150  NEXT
15160 XS = 260 / X3:YS = 170 / Y3: REM SCALE X&Y TO APPLE SCREEN
15170  IF XS > YS THEN SC = YS: REM  SCALE FACTOR FOR X & Y DATA
15180  IF XS < YS THEN SC = XS: REM  SCALE FACTOR FOR X & Y DATA
15190 SC = SC * .9: REM  SCREEN FUDGE FACTOR
15200 YO = Y3 * SC: REM  Y OFFSET FACTOR
15210 YO = YO + .05 * YO
15220 :
15230 OK = 1: REM  FLAG TO PLOT FITTED CIRCLE
15240  HGR2 : HCOLOR= 3: SCALE= 1: ROT= 0
15250  FOR A = 1 TO D(0) STEP 2
15255  IF MID = 1 THEN 15270
15260  IF A > D(0) / 2 THEN MID = 1: SCALE= 5: REM PASSED MIDDLE OF DATA SET
15270  DRAW 1 AT D(A) * SC,YO - (D(A + 1) * SC): SCALE= 1
15290  NEXT
15295 MID = 0
15300  HPLOT 0,YO TO 279,YO
15310  GOSUB 15960
15320 :
15330  GOSUB 15360
15340  GOTO 15330
15350 :
15360 FLAG = 0
15380  HOME : PRINT "FILE: ";FI$;" HAS ";D(0) / 2;" (X,Y) POINTS"
15390  VTAB 4: HTAB 5: PRINT "PREVIOUS POINTS WERE ";F;" & ";L: VTAB 6: HTAB 3: PRINT
     "ENTER FIRST AND LAST POINTS FOR": PRINT : HTAB 6: PRINT "CURVE SEGMENT <";F$;"
     ,";L$;">  ";
15394  GOSUB 15860
15396 F =  VAL (F$):L =  VAL (L$)
15400  IF F > D(0) / 2 THEN F$ = "":L$ = "": GOTO 15390
15410  IF L > D(0) / 2 THEN F$ = "":L$ = "": GOTO 15390
15420 XP = (D(L * 2 - 1) + D(F * 2 - 1)) / 2: REM X VALUES
15430 YP = (D(L * 2) + D(F * 2)) / 2: REM Y VALUES
```

```
15440 M = (D(F * 2 - 1) - D(L * 2 - 1)) / (D(L * 2) - D(F * 2))
15450 USUM = 0:LSUM = 0:Q = 0
15460  FOR I = F TO L
15470 T1 = D(I * 2 - 1) - D(L * 2 - 1) + M * (D(I * 2) - D(L * 2))
15480 USUM = USUM + T1 * ((D(I * 2 - 1) - D(L * 2 - 1)) * (D(I * 2 - 1) - D(F * 2 -
     1)) + (D(I * 2) - D(L * 2)) * (D(I * 2) - D(F * 2)))
15490 LSUM = LSUM + T1 * T1
15510  NEXT I
15513 RHO = USUM / 2 / LSUM
15515  FOR I = F TO L
15517 Q = Q + ((D(I * 2 - 1) - XP - RHO) ^ 2 - (D(L * 2 - 1) - XP - RHO) ^ 2 + (D(I *
     2) - YP - M * RHO) ^ 2 - (D(L * 2) - YP - M * RHO) ^ 2)
15520  NEXT
15530 T1 =  SQR ((D(L * 2 - 1) - XP - RHO) ^ 2 + (D(L * 2) - YP - M * RHO) ^ 2 - ( -
     YP - M * RHO) ^ 2)
15540 T2 = XP + RHO
15550 R =  SQR ((D(L * 2 - 1) - XP - RHO) ^ 2 + (D(L * 2) - YP - M * RHO) ^ 2): REM
      Circle radius
15552  FOR I = L * 2 - 1 TO F * 2 - 1 STEP  - 2:CC = I
15553  IF (D(I) > T2) THEN I = 1
15554  NEXT
15555  IF C = 78 THEN  GOTO 15660
15556 PTR = 0: REM  PRINTER FLAG OFF
15560  PRINT : IF PTR THEN  PRINT  CHR$ (4);"PR#1": PRINT : PRINT : PRINT "File: ";F
     I$;" has ";D(0);" data points": PRINT "Used data between points ";F;" and ";L: PRINT

15570  PRINT "BULK RES          =  ";T2 - T1
15580  PRINT "Rb + Rg           =  ";T2 + T1
15590  PRINT : PRINT "Radius             =  ";R: PRINT "Rel error          =  "; INT (
      SQR ( ABS (Q)) / ((L + 1 - F) * R) * 1000 + .5) / 10;" %"
15600  PRINT : PRINT "1/(Rb + Rg)        =  ";1 / (T2 + T1)
15610  PRINT "1/Bulk            =  ";1 / (T2 - T1): PRINT
15620  PRINT "MAX IMAGINARY Z   =  "; SQR ( ABS (R ^ 2 - (T2 - XP - RHO) ^ 2)) + YP +
     (M * RHO)
15623  IF 2 * F > CC THEN  PRINT "MAX IMAG Z = ";: INVERSE : PRINT "Use smaller firs
     t point": NORMAL : PRINT  CHR$ (7): GOTO 15630
15625  PRINT "FREQ. AT MAX Z    =  ";LF * (10 ^ (MM * ((CC - 1) / 2 + ((D(CC) - T2) /
     (D(CC) - D(CC + 2))))));: PRINT " KHz"
15630  PRINT "DEPRESSED ANGLE   =  "; ATN ( SQR (R ^ 2 - T1 ^ 2) / T1) * 57.2957796;
     " DEG"
15635  IF PTR THEN PTR = 0: PRINT D$;"PR#0": GOTO 15360
15640  VTAB 24: HTAB 5: PRINT "HIT ANY KEY TO CONTINUE ... ";: GET A$: PRINT
15650 :
15660 C = 0: POKE  - 16299,0: POKE  - 16304,0
15662 :
15663  REM  +---------------------+
15664  REM  !     PLOT  CIRCLE    !
15665  REM  +---------------------+
15666 :
15668 I = 0
15670  FOR X = (T2 - T1) TO (T2 + T1) STEP T1 / 20: REM ABOUT 40 STEPS AROUND HALF C
     IRCLE
15680 Y =  SQR ( ABS (R ^ 2 - (X - XP - RHO) ^ 2)) + YP + (M * RHO)
15682 I = I + 1
15684 X(I) = X:Y(I) = Y
15690  IF X = (T2 - T1) THEN XF = X:YF = Y
15700  IF X > T2 AND FLAG = 0 THEN XM = X:YM = Y:FLAG = 1
15705  IF ( ABS (X * SC) > 279) OR ( ABS (YO - (Y * SC)) > 189) THEN  NEXT
```

```
15710  DRAW 2 AT  ABS (X * SC), ABS (YO - (Y * SC)): IF  NOT OK THEN  XDRAW 2
15720  NEXT
15750  REM  ! PLOT CIRCLE CENTRE !
15780 XQ = (XF + XM) / 2:YQ = (YF + YM) / 2
15790  DRAW 3 AT T2 * SC,YO - SC * (YQ - ((XM - XF) / (YM - YF)) * (T2 - XQ)): IF  NOT
     OK THEN  XDRAW 3: REM  Circle Centre
15792  SCALE= 1
15800 F$ = "":L$ = ""
15803 :
15805  TEXT
15810 CHECK = 1: VTAB 23: PRINT  CHR$( 40);: HTAB 10: PRINT " OK ? (Y/N) ";
15812  GOSUB 15860
15840  GOTO 15810
15850  RETURN
15860  GET C$:C =  ASC (C$): IF C = 13 THEN COMMAS = 0: RETURN
15862  IF C = 27 THEN  POP : POP : GOTO 40
15870  IF C = 7 THEN  GOSUB 15950
15875  IF C = 16 THEN PTR = 1: POP : GOTO 15560
15877  IF C = 17 THEN SN% = 1:XX =  PEEK (54):YY =  PEEK (55): POKE 54,0: POKE 55,19
     2 + SN%: CALL 25091: POKE 55,YY: POKE 54,XX
15880  IF C = 20 THEN  GOSUB 15960
15885  IF C = 23 THEN  GOSUB 16000
15890  IF CHECK AND C < 31 THEN  POP : GOTO 15810
15892  IF  NOT CHECK AND C < 31 THEN  POP : GOTO 15360
15900  IF C = 44 THEN COMMAS = 1
15910  IF C > 47 AND C < 58 AND COMMAS = 0 THEN F$ = F$ + C$
15920  IF C > 47 AND C < 58 AND COMMAS = 1 THEN L$ = L$ + C$
15922  IF C = 89 THEN OK = 1: POP : GOTO 15360
15924  IF C = 78 THEN OK = 0:FLAG = 0: POP : GOTO 15420
15930  POP : GOTO 15360
15950  POKE  - 16304,0: POKE  - 16299,0: RETURN
15960  POKE  - 16300,0: POKE  - 16303,0: RETURN
16000 :
16010  REM  Write fitted file
16015 ZA = ZA + 1
16020  PRINT : PRINT  CHR$ (4);"OPEN";FI$;".FIT/"ZA",D2"
16030  PRINT  CHR$ (4);"WRITE";FI$;".FIT/"ZA
16035  PRINT 80
16040  FOR I = 1 TO 40
16050  PRINT X(I): PRINT Y(I)
16060  NEXT
16070  PRINT  CHR$ (4);"CLOSE";FI$;".FIT/"ZA
16080  RETURN
17000  REM  List program
17005  PRINT  CHR$ (4);"PR#1"
17010  PRINT  CHR$ (27)"M" CHR$ (9)"90N" CHR$ (27)"N" CHR$ (8)
17020  LIST
17030  PRINT  CHR$ (4);"PR#0"
17040  END
```

Appendix B

VARIABLES USED IN MAIN PROGRAM*

A	140	Value of A$ - response to a general GET statement
A$	140	Response to a general GET statement
	2300	- also input of real part from HP 4192A spectrometer
A${*}	50	Sample ID information
AA$	1740	Response to a general GET statement
B$	2300	Input of imaginary part from HP 4192A spectrometer
BL$	2440	Bell
C	15555	Value of general GET statement in line 15860
C$	15860	Response to general GET statement
CC	15552	Counter - set to I after passing circle centre {T2} on scanning around semicircle.
CHECK	15810	Flag set if passed through line 15810, i.e., figure has been plotted already {may wish to delete}
COMMAS	15860	Flag set if response to GET {C$, 15860} is a comma, i,e, switch further GET input from first {F$} to last {L$} subscript ranges of data used to fit circle.
D$	32	Ctrl-D for disc i/o through DOS
D{*}	50	Single dimensional array for data
DA	2170	Device address for IEEE-488 bus access to HP-4192A
DL$	2180	Device listen
DT$	2180	and device talk address for HP-4192A
E	1830	Flag - set if data returned in scientific notation. Used to subsequently split {and discard} the insignificant part of the mantissa from the exponent for formatting output to a printer.
ER	2440	Value of error code returned from PEEK{222}
F	15390	Value of present first data point used to fit circle
F$	15390	Value of previous first data point used to fit circle
FI$	590	File name used to store and recall data
FLAG	15360	Flag - set if passed centre of circle - hence mid-point values of X and Y {XM,YM} can be determined between first {X,Y} pair and first {X,Y} pair passed top of circle ... through which a perpendicular is drawn that passes through circle centre.
FR	2122	Frequency at which data A$,B$ obtained from HP-4192A.
FR$	2130	String form of FR
HF	320	High frequency limit for scan
HT$	1340	Horizontal tab key for printer
I	440	General counter
IC	2590	Variable used to check for present of IEEE-488 card

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* Listing is for complete program, i.e, that given in ref. 1 and the subroutine given in Appendix I of this report.

J	880	General counter
L	1840	Length of string containing numerical values sent to printer
L$	15390	String containing value of Last datum in array through which circle will be fitted
LF	320	Low frequency limit for scan
LSUM	15450	Denominator in equation {14} used to determine Rho
M	15440	Slope of line AB
MM	320	Number of points/decade used in log{frequency} scan
N	90	Number of values on screen when listing data {line 480}
OK	15220	Flag - if set {1}, plot fitted circle; if not, erase previous fitted points
P2	1600	Pi x 2 - used to determine Capacitance {1/2pi.f.X}
PTR	15556	Flag - if set, printer on
Q	15450	Sum of differences between actual data and fitted curve
R	15550	Radius of circle
RHO	15513	Distance along radius from centre {AB}
SC	15170	Scale factor used to fit data on graphics screen
SL	50	Back plane slot holding IEEE card
T$	32	Ctrl-Z - terminator for statements on IEEE bus
T1	15470	Half distance in X across circle at Y=0
T2	15540	X co-ordinate for circle centre
USUM	15450	Numerator in equation {14} used to determine Rho
X	1180	General counter
X{*}	50	Array holding X co-ordinates for fitted circle
X1	90	Number of screens {20 lines each} of data listed to screen
X3	15080	Maximum value of X
XF	15690	Value of X for first datum through which circle is fitted
XM	15700	First value of X greater than T2 in traversing around fitted circle data from D{F} to D{L}
XP	15420	Xprime - at point B in Fig. 1
XS	15160	X scale factor to fit data to graphics screen
Y	1550	Impedance, Admittance, Capacitance, Dissipation values sent to printer
Y{*}	50	Array holding Y co-ordinates for fitted circle
Y3	15120	Maximum value Y
YF	155690	Value of Y for first datum though which circle is fitted
YM	15700	Value of Y at XM
YO	15200	Y-axis offset
YP	15430	Yprime - at point B in Fig. 1
YS	15160	Y scale factor to fit data to graphics screen
ZZ	340	Flag - if set, then IEEE bus is dead